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The $\pi^+\pi^+$ scattering length from maximally twisted mass lattice QCD

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Abstract

We calculate the s-wave pion-pion scattering length in the isospin $I = 2$ channel in lattice QCD for pion masses ranging from 270 MeV to 485 MeV using two flavors of maximally twisted mass fermions at a lattice spacing of 0.086 fm. Additionally, we check for lattice artifacts with one calculation at a finer lattice spacing of 0.067 fm. We use chiral perturbation theory at next-to-leading order to extrapolate our results. At the physical pion mass, we find $m_\pi a_{\pi\pi}^{I=2} = -0.04385\,(28)(38)$ for the scattering length, where the first error is statistical and the second is our estimate of several systematic effects.

Key words: pion-pion scattering length, lattice QCD
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1 Introduction

In the limit of massless up and down quarks, the resulting chiral symmetry of QCD is spontaneously broken and consequently the meson spectrum contains

three massless Goldstone bosons, $\pi^{\pm}$ and π^0. Due to the unique role played by the pions, their interactions are strongly determined by the underlying chiral symmetry, and the s-wave pion-pion scattering lengths even vanish in the chiral limit. Thus the scattering lengths are sensitive to the chiral dynamics of the strong interactions, and the non-perturbative calculation thereof, the subject of this paper, is an integral part of understanding the low energy properties of QCD.

In nature, the masses of the quarks are not zero but small and induce an explicit but weak breaking of chiral symmetry. Correspondingly, the pions are not massless but light. This breaking of chiral symmetry is systematically treated in chiral perturbation theory (χPT) by considering the quark masses as perturbations. Furthermore, the pion-pion scattering lengths no longer vanish and at leading order (LO) in χPT are predicted by Weinberg [1] solely in terms of the pion mass, m_π, and the pion decay constant, f_π, as

$$m_\pi a_{\pi\pi}^{I=0} \approx \frac{7m_\pi^2}{16\pi f_\pi^2} = 0.160\,(1) \quad \text{and} \quad m_\pi a_{\pi\pi}^{I=2} \approx -\frac{m_\pi^2}{8\pi f_\pi^2} = -0.0456\,(1)\,,$$

where $a_{\pi\pi}^{I=0}$ and $a_{\pi\pi}^{I=2}$ denote the isospin $I = 0$ and $I = 2$ s-wave scattering lengths respectively. The next-to-leading order (NLO) corrections depend on unknown low energy constants, which can be determined from experimental measurements or lattice calculations.

The experimental measurement of $K^{\pm} \to \pi^+\pi^-e^{\pm}\nu$ (K_{e4}) decays by E865 at BNL [2] gives

$$m_\pi a_{\pi\pi}^{I=0} = 0.203\,(33) \quad \text{and} \quad m_\pi a_{\pi\pi}^{I=2} = -0.055\,(23)\,.$$

When combined with constraints from χPT, these measurments yield

$$m_\pi a_{\pi\pi}^{I=0} = 0.216\,(14) \quad \text{and} \quad m_\pi a_{\pi\pi}^{I=2} = -0.0454\,(34)\,.$$

A combination of several experimental and theoretical inputs from CGL [3,4] produces a consistent but more precise result of

$$m_\pi a_{\pi\pi}^{I=0} = 0.220\,(5) \quad \text{and} \quad m_\pi a_{\pi\pi}^{I=2} = -0.0444\,(10)\,.$$

Additionally, the recent measurments of K_{e4} decays [5] and $K^{\pm} \to \pi^{\pm}\pi^0\pi^0$ decays [6] by NA48/2 at CERN [7] give, without making any use of χPT constraints,

$$m_\pi a_{\pi\pi}^{I=0} = 0.221\,(5) \quad \text{and} \quad m_\pi a_{\pi\pi}^{I=2} = -0.0429\,(47).$$

Including χPT in their analysis, NA48/2 finds [8]

$$m_\pi a_{\pi\pi}^{I=0} = 0.220\,(3) \quad \text{and} \quad m_\pi a_{\pi\pi}^{I=2} = -0.0444\,(9).$$

The results are all consistent with each other and the most precise results from NA48/2 are in agreement with the lattice results given shortly.

The non-perturbative determination of the scattering lengths from lattice QCD is possible, despite the Euclidean nature of the calculation, by using a finite size method due to Lüscher [9–13]. This method capitalizes on the relationship between the energy eigenvalues of a two pion system enclosed in a finite spatial box and the scattering phase of two pions in infinite volume. In the derivation of this result, it is assumed that the physical box size is large enough to avoid significantly altering the two pion interaction. In this limit, the intrinsic finite size effects of each individual pion are exponentially suppressed. The dominant contribution to the finite size dependence of a two pion state is then simply given by the interaction between the two pions due to the finite volume. Thus the strength and nature, repulsive or attractive, of the interaction of two pions will shift the energies of the otherwise free pions. This shift then relates the energy eigenvalues to the scattering phase and ultimately the scattering lengths of two pions.

One obstacle to the lattice determination of the pion-pion scattering lengths is the presence of disconnected diagrams that render the calculation of the $I = 0$ channel computationally demanding. On the other hand, the simpler $I = 2$ channel does not require such diagrams and consequently many lattice groups have focused their efforts on this case. Furthermore, most calculations of the scattering lengths to date have been carried out within the quenched approximation [14–35]. There have been only two previous calculations of $a_{\pi\pi}^{I=2}$ with dynamical fermions. The first such calculation was performed by CP-PACS with $N_f = 2$ tadpole-improved clover fermions at rather heavy pion masses in the range $m_\pi = 0.5$ GeV to 1.1 GeV [36]. However, it is doubtful that χPT at NLO, or any order, can be applied to such heavy pion masses. The other full QCD calculation was performed by NPLQCD with domain-wall valence quarks on the $N_f = 2 + 1$ asqtad-improved coarse MILC ensembles with $m_\pi = 290$ MeV to 590 MeV [37,38]. Mixed-action χPT at NLO was used to perform the chiral and continuum extrapolations. At the physical pion mass, NPLQCD finds

$$m_\pi a_{\pi\pi}^{I=2} = -0.04330\,(42) \quad \text{and} \quad l_{\pi\pi}^{I=2}(\mu = f_{\pi,\text{phy}}) = 6.2\,(1.2)\,,$$

where $l_{\pi\pi}^{I=2}(\mu)$ is a low energy constant (LEC) appearing in the χPT description of the quark mass dependence of the scattering length. As discussed later, $l_{\pi\pi}^{I=2}(\mu)$ is evaluated at $\mu = f_{\pi,\text{phy}}$, where $f_{\pi,\text{phy}}$ is the physical value of the

pion decay constant.

In this work we determine the s-wave $I = 2$ pion-pion scattering length and the corresponding $l_{\pi\pi}^{I=2}$ by using the $N_f = 2$ maximally twisted mass fermion ensembles from the European Twisted Mass Collaboration (ETMC). Our lightest pion mass is lighter than those of the previous calculations and allows us to further probe the chiral limit. Due to the properties of twisted mass fermions at maximal twist, our calculation is automatically accurate to $O(a^2)$ in the lattice spacing, a. Additionally, we perform an explicit check for large lattice artifacts with a single calculation at a finer lattice spacing. As presented later, we find at the physical pion mass

$$m_\pi a_{\pi\pi}^{I=2} = -0.04385\,(28)(38) \quad \text{and} \quad l_{\pi\pi}^{I=2}(\mu = f_{\pi,\text{phy}}) = 4.65\,(.85)(1.07)\,,$$

which is in agreement with the above experimental measurements and phenomenological analysis as well as the previous lattice calculation.

2 Method

2.1 Lüscher's finite size method

As mentioned in the introduction, Lüscher's finite size method relates the energy levels of two pion states in a finite volume to the scattering phase in the infinite volume. For the case of two pions with zero total three-momentum, this method establishes a relationship between the lowest energy eigenvalue $E_{\pi\pi}^I$ with a given isospin I in a finite box of size L and the corresponding scattering length $a_{\pi\pi}^I$. For the $I = 2$ channel, it is given in Ref. [10] as

$$\begin{aligned}\delta E_{\pi\pi}^{I=2} &= E_{\pi\pi}^{I=2} - 2m_\pi \\ &= -\frac{4\pi a_{\pi\pi}^{I=2}}{m_\pi L^3}\left[1 + c_1\frac{a_{\pi\pi}^{I=2}}{L} + c_2\left(\frac{a_{\pi\pi}^{I=2}}{L}\right)^2\right] + O(L^{-6})\,,\end{aligned} \tag{1}$$

where $c_1 = -2.837297$ and $c_2 = 6.375183$ are numerical constants. Thus the above result allows us to convert a lattice determination of the energy shift, $\delta E_{\pi\pi}^{I=2}$, into a calculation of $a_{\pi\pi}^{I=2}$.

2.2 Extraction of $\delta E_{\pi\pi}^{I=2}$

To extract $\delta E_{\pi\pi}^{I=2}$, we construct the π^+ and $\pi^+\pi^+$ two-point correlation functions from the operators proposed in Ref. [24],

$$C_\pi(t) = \langle (\pi^+)^\dagger (t+t_s) \pi^+(t_s) \rangle$$

and

$$C_{\pi\pi}(t) = \langle (\pi^+\pi^+)^\dagger (t+t_s)(\pi^+\pi^+)(t_s) \rangle \, .$$

Here t_s is an arbitrary time slice, $\pi^+(t) = \sum_{\vec{x}} (\bar{d}\gamma_5 u)(\vec{x},t)$ is an interpolating operator for the π^+ meson with zero total three-momentum and $(\pi^+\pi^+)(t)$ is an interpolating operator for the two pion state, again with zero total three-momentum, given by

$$(\pi^+\pi^+)(t) = \pi^+(t+a)\pi^+(t) \, .$$

In order to avoid complications due to Fierz rearrangement of quark lines as discussed in Ref. [24], we use the π^+ interpolating fields at time slices separated by one lattice spacing.

From the large time behavior of $C_\pi(t)$ and $C_{\pi\pi}(t)$, it is possible to extract the corresponding ground state energies as follows,

$$C_\pi(t) \to A_\pi \exp(-m_\pi \, t) \quad \text{and} \quad C_{\pi\pi}(t) \to A_{\pi\pi} \exp(-E_{\pi\pi}^{I=2} \, t) \, ,$$

where we assume that t is large enough to neglect excited states but still far enough from the boundaries to ignore boundary effects. Furthermore, constructing the following ratio of correlation functions we can determine $\delta E_{\pi\pi}^{I=2}$ directly as

$$\frac{C_{\pi\pi}(t)}{C_\pi^2(t)} \to \frac{A_{\pi\pi}}{A_\pi^2} \exp(-\delta E_{\pi\pi}^{I=2} \, t)$$

where t satisfies the same requirements as before. However, we use anti-periodic boundary conditions for the quarks in the time direction in order to match the sea quarks used in our calculation, and this leads to a more complicated time dependence for C_π and $C_{\pi\pi}$.

2.3 Anti-periodic boundary conditions

As mentioned above, in our calculation we employ anti-periodic boundary conditions in the time direction for the fermions. Using the transfer matrix formalism, the time dependence of our correlation functions is given by

$$\langle O^{\dagger}(t)O(0)\rangle = \mathrm{Tr}\left(e^{-H(T-t)}O^{\dagger}(0)e^{-Ht}O(0)\right)/\,Z\,,$$

where the time-slice transfer matrix is e^{-aH}, the partition function Z is given by $Z = \mathrm{Tr}(e^{-HT})$ where T is the total time extent of our lattice and $O(t)$ represents either $\pi^+(t)$ or $(\pi^+\pi^+)(t)$. Inserting a complete set of eigenstates of H into the above equation yields

$$\begin{aligned}\langle O^{\dagger}(t)O(0)\rangle &= \sum_{m,n}|\langle n|O|m\rangle|^2 e^{-E_m(T-t)}e^{-E_n t}/\,Z\\ &= \sum_{m,n}|\langle n|O|m\rangle|^2 e^{-(E_m+E_n)T/2}\cosh((E_m-E_n)(t-T/2))/\,Z\,.\end{aligned}$$

The terms in the above series are thermally suppressed by factors of e^{-E_mT} or e^{-E_nT}. Only those terms with $E_m = 0$ or $E_n = 0$ remain in the zero temperature, $T \to \infty$, limit. However, the effects of the suppressed contributions can still distort the behavior of correlation functions for finite values of T, particularly in the large t region.

This phenomenon does indeed occur in this work for the two pion operator. Intermediate states $\langle n| = \langle \pi^+|$ and $\langle m| = \langle \pi^-|$ give a constant, in t, contribution to $C_{\pi\pi}$,

$$|\langle \pi^+|\pi^+\pi^+|\pi^-\rangle|^2 e^{-m_\pi T}/Z\,.$$

This is comparable to the standard contribution,

$$|\langle \pi^+\pi^+|\pi^+\pi^+|\Omega\rangle|^2 e^{-E_{\pi\pi}^{I=2}T/2}\cosh(E_{\pi\pi}^{I=2}(t-T/2))/Z\,,$$

when t approaches $T/2$. To be precise, for large enough volumes $E_{\pi\pi}^{I=2} = 2m_\pi + \delta E_{\pi\pi}^{I=2} \approx 2m_\pi$, and hence these two contributions to $C_{\pi\pi}$, $e^{-m_\pi T}$ and $e^{-E_{\pi\pi}^{I=2}T/2}\cosh(E_{\pi\pi}(t-T/2))$ are in fact nearly equal for $t = T/2$. Additionally, the factor $C_\pi(t)^2$ has similar problems. The correlator $C_\pi(t)$ itself has a simple spectral representation. However, the square is more complicated and also contains a constant, in t, contribution as well.

To eliminate these contaminations, we use the derivative method [39] and define a modified ratio, $R(t)$, in the following way

$$R(t+a/2) = \frac{C_{\pi\pi}(t) - C_{\pi\pi}(t+a)}{C_\pi^2(t) - C_\pi^2(t+a)}\,. \tag{2}$$

The asymptotic form for $R(t)$, ignoring terms suppressed relative to the leading contribution, is

$$R(t+a/2) = A_R\left(\cosh(\delta E_{\pi\pi}^{I=2}\,t') + \sinh(\delta E_{\pi\pi}^{I=2}\,t')\,\coth(2m_\pi t')\right) \tag{3}$$

where A_R is a combination of amplitudes in C_π and $C_{\pi\pi}$ and $t' = t+a/2-T/2$. Since m_π is the most accurately calculated component of our calculation, $R(t)$ provides a nearly direct determination of $\delta E_{\pi\pi}^{I=2}$ and cleanly eliminates the unwanted thermal contributions that spoil the simple ratio given earlier.

3 Lattice Calculation

3.1 *Twisted mass fermions*

In this work we use the two flavor maximally twisted mass fermion configurations from ETMC. Using twisted mass fermions at maximal twist ensures that physical observables are automatically accurate to $O(a^2)$ in the lattice spacing [40]. Most of the results presented here are from a sequence of ensembles with a lattice spacing of $a = 0.086$ fm and a box size of $L = 2.1$ fm. The pion masses range from $m_\pi = 270$ MeV to 485 MeV. For the lower pion masses the volume is increased to $L = 2.7$ fm, and there is one calculation using a finer lattice spacing of $a = 0.067$ fm. The parameters relevant to this calculation are given in Tab. 1, and further details can be found in Refs. [41–43].

3.2 *Stochastic sources*

For the calculation of pion correlation functions, it is known that the stochastic source method is more efficient than the point source method. Therefore, in the present work, we employ Z_4 stochastic noise with two noise sources generated on each source time slice. Since we place the source on two time slices for the $\pi^+\pi^+$ correlation function, t_s and $t_s + a$, we therefore perform four inversions for each configuration. We remark that we also use the one-end trick in this work for the evaluation of correlation functions [44–46] leading to a further

β	$a\mu$	L/a	m_π	m_π/f_π	N	$a\delta E_{\pi\pi}^{I=2}\cdot 10^3$	$m_\pi a_{\pi\pi}^{I=2}$
3.90	0.0100	24	485	2.77(2)	479	7.23(59)(41)	-0.297(20)(16)
3.90	0.0085	24	448	2.61(1)	487	7.66(65)(33)	-0.269(17)(10)
3.90	0.0064	24	391	2.40(1)	553	9.6(1.3)(.6)	-0.252(22)(13)
3.90	0.0040	32	309	2.02(1)	490	3.96(36)(22)	-0.165(14)(08)
3.90	0.0030	32	270	1.85(1)	562	4.05(42)(21)	-0.130(12)(06)
4.05	0.0030	32	307	2.08(2)	375	7.1(1.2)(.9)	-0.171(18)(22)

Table 1
Ensembles used in this work. Only dimensionless quantities are needed in this calculation, but for guidance we give the value of m_π rounded to the nearest MeV for each ensemble indicated by β, $a\mu$ and L/a. We also list the ratio m_π/f_π, the number, N, of configurations used, the energy shift $a\delta E_{\pi\pi}^{I=2}$ and the scattering length $m_\pi a_{\pi\pi}^{I=2}$. The first uncertainty is statistical and, when present, the second one is systematic.

improvement in the signal-to-noise ratio. Additionally, the source time slices, t_s, are chosen randomly to reduce the autocorrelation between consecutive trajectories.

4 Results

4.1 Calculation of $m_\pi a_{\pi\pi}^{I=2}$

In Fig. 1 we show our lattice results for $R(t)$, defined in Eq. 2, as a function of the time t together with a correlated fit to the asymptotic form given in Eq. 3. All the ensembles shown in Fig. 1 visibly agree with the corresponding fit and lead to reasonable values of χ^2 per degree of freedom (dof), where χ^2 is the correlated figure-of-merit function. To further verify these fits, we examined several possible sources of systematic error. First, the ratio could suffer from bias at large t, so we examined the jackknife estimate of bias but found it to be significantly smaller than the errors for all the ensembles. Second, we considered the possibility that we underestimated the errors due to autocorrelations. However, both the gamma method [47] and standard binning showed no significant signs of autocorrelation for $R(t)$ in any of the ensembles. The possibility of π^0 mixing, due to the breaking of parity at non-zero lattice spacing for twisted mass fermions, is considered in Sect. 4.2. But as described there in more detail, we find no statistically significant indications of the π^0 contributions.

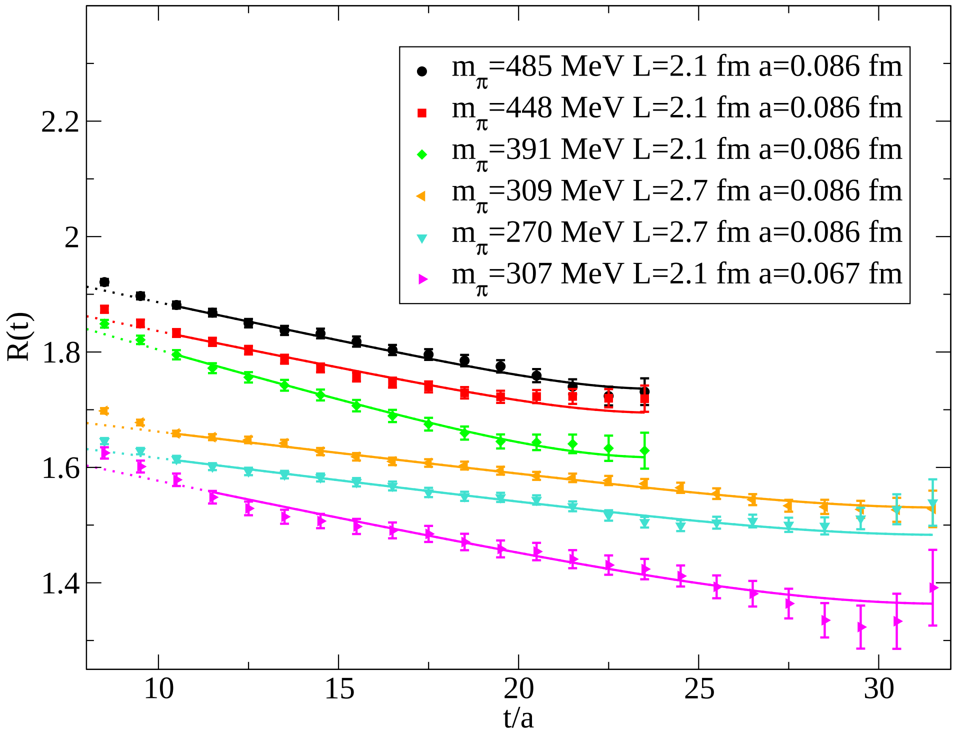

Fig. 1. The ratio $R(t)$ as a function of t. The solid lines are correlated fits to Eq. 3, from which the energy shifts $a\delta E_{\pi\pi}^{I=2}$ are extracted. The ensembles have been shifted vertically to facilitate easier comparison.

There is one further possible systematic error due to the contributions from excited states in the small t region or from unphysical π^0 states in the large t region. To ensure that the fits for these ensembles are safe from such effects, we study the systematic errors caused by choosing a fitting window in which to match to the asymptotic form for $R(t)$. First we ensure that the results exhibit clear plateaus when we increase the minimum t or decrease the maximum t used in the fits. However, to provide a quantitative estimate of the systematic error, we perform the following distribution method. We collect the results for $a\delta E_{\pi\pi}^{I=2}$ from all fitting intervals with $\chi^2/\mathrm{dof} < 2$. This includes varying both the minimum and maximum time extent for the fitting range and results in 30 to 60 values of $a\delta E_{\pi\pi}^{I=2}$ for each ensemble. We then make the distribution of these selected results and choose the median of this distribution for the central value. Then we take the central, and symmetric about the median, 68% region of the distribution to define the systematic error. Finally, we use the jackknife method to determine the statistical error on the central values. This method is also applied to $m_\pi a_{\pi\pi}^{I=2}$, and the results for $a\delta E_{\pi\pi}^{I=2}$ and $m_\pi a_{\pi\pi}^{I=2}$ are given in Tab. 1. As shown in this table, the resulting estimates of the systematic errors are typically smaller than the corresponding statistical errors, and are at worst of the same order as the statistical errors. Since the distribution method used to estimate the systematic errors is itself subject to statistical errors, this is precisely what is expected if there are no substantial systematic

effects. However, since the final statistical precision for the value of $m_\pi a_{\pi\pi}^{I=2}$ at the physical limit turns out to be quite small, we decided, in order to avoid underestimating our final error, to carefully propagate these systematic errors through to the final result as described later in Sect. 4.5.

4.2 π^0 contamination

Twisted mass fermions violate parity and isospin at non-zero values of the lattice spacing. Therefore the spectral representation of the π^+ and $\pi^+\pi^+$ correlators can admit states that would not be present in the continuum limit. In particular, unphysical contributions from the π^0, which has a mass m_{π^0} different, and smaller, than the mass m_π of the $\pi^\pm$, may enter the C_π and $C_{\pi\pi}$ correlators in several ways [46]. Furthermore, these effects are believed to be more noticable in pion-pion scattering, so the successful calculation of all three isospin channels, $I = 0$, 1 and 2, would test the twisted mass formulation of lattice QCD.

The π^0 can enter the C_π correlator through intermediate states of the form $\langle\pi^+|\pi^+|\pi^0\rangle$ and $\langle\pi^+\pi^0|\pi^+|\Omega\rangle$. The former contribution is thermally suppressed by a factor of $e^{-m_{\pi^0}T}$, however it leads to a time dependence with an energy of $m_\pi - m_{\pi^0}$ that is lighter than the usually expected m_π ground state. The second contribution is not thermally suppressed but corresponds to the first excited state with energy $E_{\pi^+\pi^0} \approx m_\pi + m_{\pi^0}$. This is lighter than the first physical excited state with energy near $3m_\pi$. Similarly, $C_{\pi\pi}$ contains unphysical contributions from $\langle\pi^+\pi^+|\pi^+\pi^+|\pi^0\rangle$ and $\langle\pi^+\pi^+\pi^0|\pi^+\pi^+|\Omega\rangle$. Again there is an additional light state that is thermally suppressed by $e^{-m_{\pi^0}T}$ but has an energy of $E_{\pi^+\pi^+} - m_{\pi^0} \approx 2m_\pi - m_{\pi^0}$ that is lower than the physical ground state near $2m_\pi$, and the first excited state is lowered to $E_{\pi^+\pi^+\pi^0} \approx 2m_\pi + m_{\pi^0}$ rather than the expected energy of approximately $2\sqrt{m_\pi^2 + (2\pi/L)^2}$.

The parity violating matrix elements responsible for these effects are $O(a)$ in the lattice spacing, even at maximal twist, however the matrix elements appear squared in the correlators. Therefore these unphysical states make an $O(a^2)$ contribution. The question, however, is not about the scaling in the lattice spacing, but about the size of this contribution at the lattice spacings used in this work. A detailed discussion of this issue can be found in Ref. [48]. Here, our focus is more practical. We want to ensure that the scattering lengths calculated in this work are not significantly distorted due to these effects.

First, the naive estimate for the suppression factor for the additional light contributions, $m_\pi - m_{\pi^0}$ in C_π and $E_{\pi^+\pi^+} - m_{\pi^0}$ in $C_{\pi\pi}$, is $(a\Lambda_{\rm QCD})^2 e^{-m_{\pi^0}T}$. The value of m_{π^0} is difficult to calculate precisely, but it is clear from Ref. [48] that m_{π^0} is never more than 20% lighter than m_π for the ensembles in this

work. Therefore we will simply use m_π and a value of $\Lambda_{\rm QCD} = 250$ MeV to set the order of magnitude for these suppression factors. We find that for the ensembles used here, the largest value of $(a\Lambda_{\rm QCD})^2 e^{-m_{\pi^0}T}$ is $9 \cdot 10^{-6}$ for the $\beta = 4.05$, $a\mu = 0.0030$ ensemble in Tab. 1. Using the actual value of m_{π^0} from [48] raises this to $2 \cdot 10^{-5}$. This value is small, but it is not too far beyond the statistical precision of the correlators used to calculate $a\delta E_{\pi\pi}^{I=2}$, hence we must carefully check for these contributions.

Second, there are the additional states that are only suppressed by $(a\Lambda_{\rm QCD})^2$. However, these states are heavier than the physical state and hence would occur in the correlators as excited states. The naive suppression factors are $1 \cdot 10^{-2}$ and $7 \cdot 10^{-3}$ for $a = 0.086$ fm and 0.067 fm respectively. These simple estimates are larger than for the other states, however these contributions are also more strongly suppressed by their own energies.

In the light of these arguments, we made a significant effort to attempt to find such effects anyway. We tried fitting the individual $C_\pi(t)$ and $C_{\pi\pi}(t)$ correlators as well as the ratio $R(t)$ to various functional forms including the physical state and both the additional heavier and lighter states, just the lighter state or just the heavier state. We fit the most general forms, keeping all energies as free parameters, and additionally constrained forms, in which we constrained m_{π^0} based on known values. And we also explored several minimization methods. The net result was that one could indeed lower the χ^2 value for each fit, but the χ^2 per degree of freedom still increased, indicating no statistically significant contribution from the unwanted π^0 states.

However, we must offer a few words of caution. While we could not find any compelling evidence for these contributions, we of course can not rule out their presence at a level beneath our statistical resolution. We should further note that there are visible excited states in the correlators. However, the accuracy of the correlators for the ensembles studied here does not allow us to distinguish the physical excited states, near $3m_\pi$ for C_π and $2\sqrt{m_\pi^2 + (2\pi/L)^2}$ for $C_{\pi\pi}$, from the unphysical excited states, near $m_\pi + m_{\pi^0} \approx 2m_\pi$ for C_π and $2m_\pi + m_{\pi^0} \approx 3m_\pi$ for $C_{\pi\pi}$. The extensive study of systematic errors due to the fitting range discussed in the previous section was partially motivated by these issues. It provides the quantitative statement that these effects do not rise to the level of our statistical precision and gives an estimate of the systematic error.

Additionally, there are two reasons that these contributions may be smaller than anticipated. First, the unphysical contributions correspond to scattering states that may be suppressed by a power of the volume. Second, the construction of $R(t)$ in Eq. 2 forms a discrete approximation to the ratio of derivatives of $C_{\pi\pi}$ and C_π^2 and may further suppress the nearly constant light state contributions. Finally, these effects are anticipated to be more substantial for the other isospin channels, hence a detailed understanding of the π^0 contribu-

tions to pion-pion scattering will have to await our ongoing calculations in the $I = 1$ [49] channel and our planned work for $I = 0$.

4.3 Finite volume effects

The dominant finite size effect in this calculation is, of course, the shift in $\delta E_{\pi\pi}^{I=2}$ due to the interactions of two pions in a finite volume. Additionally, there are the exponentially small, as opposed to the merely power suppressed, finite volume corrections to $I = 2$ pion-pion scattering that have been determined for scattering near threshold in Ref. [50]. The resulting finite size corrections for the scattering length are given there as,

$$(m_\pi a_{\pi\pi}^{I=2})_L = (m_\pi a_{\pi\pi}^{I=2})_\infty + \Delta_{FV}$$

where

$$\begin{aligned}\Delta_{FV} &= -\frac{m_\pi^2}{8\pi f_\pi^2}\left\{\frac{m_\pi^2}{f_\pi^2}\frac{\partial}{\partial m_\pi^2} i\Delta\mathcal{I}(m_\pi) + \frac{2m_\pi^2}{f_\pi^2} i\Delta\mathcal{J}_{exp}(4m_\pi^2)\right\} \\ &= \frac{1}{2^{13/2}\pi^{5/2}}\left(\frac{m_\pi}{f_\pi}\right)^4 \sum_{|\mathbf{n}|\neq 0} \frac{e^{-|\mathbf{n}|m_\pi L}}{\sqrt{|\mathbf{n}|m_\pi L}}\left\{1 - \frac{17}{8}\frac{1}{|\mathbf{n}|m_\pi L} + O\left(L^{-2}\right)\right\}.\end{aligned}$$

Using the above result, we calculate the corrections to $m_\pi a_{\pi\pi}^{I=2}$. Compared to the statistical errors, the finite volume corrections are negligible. To be precise, they are never more than 6% of the corresponding statistical error and are hence ignored in the following analysis.

There is a second finite size effect originating from the effective range approximantion, $p\tan^{-1}\delta(p) = 1/a_{\pi\pi}^{I=2} + \frac{1}{2}r_{\text{eff}}p^2$, which is used to relate the scattering phase $\delta(p)$ at vanishingly small momentum p to the scattering length. The dependence on the effective range r_{eff} is very small and gives rise to the corrections at $O(L^{-6})$ in Eq. 1. As argued in Ref. [38], assuming that the effective range is at most twice the scattering length, this correction can be estimated using the measured values of m_π and $\delta E_{\pi\pi}^{I=2}$. Using the result given in Ref. [38], we calculate this correction and find that it is never more than 9% of the corresponding statistical error of $m_\pi a_{\pi\pi}^{I=2}$. Hence, this finite size effect is also sufficiently small to be ignored as well.

4.4 Lattice artifacts

Most of the calculations presented here use a single lattice spacing of 0.086 fm, but we have also performed an additional calculation of $\delta E_{\pi\pi}^{I=2}$ and $m_\pi a_{\pi\pi}^{I=2}$ at a second lattice spacing of 0.067 fm and at a pion mass of 307 MeV. This pion mass lies very close to that of the $a = 0.086$ fm, $m_\pi = 309$ MeV point. The physical volumes of these two ensembles differ, so the values of $\delta E_{\pi\pi}^{I=2}$ can not be directly compared. However, assuming that Lüscher's method correctly accounts for the finite volume dependence of $\delta E_{\pi\pi}^{I=2}$ for these two ensembles, we can compare $m_\pi a_{\pi\pi}^{I=2}$ for the two lattice spacings, and indeed we do find statistical agreement between the two ensembles as indicated in Tab. 1. Furthermore, as described in the next section, we note that the expected $O(a^2)$ corrections from maximally twisted mass lattice QCD are actually weakened to $O(m_\pi^2 a^2)$ for the $I = 2$, $I_3 = \pm 2$ channel as shown using twisted mass χPT [51], thus suggesting further that the lattice spacing dependence of $m_\pi a_{\pi\pi}^{I=2}$ is mild for the calculations in this work.

4.5 Chiral extrapolation

The pion-pion scattering lengths have recently been calculated in twisted mass χPT [51]. This is an expansion of twisted mass lattice QCD in both the quark masses and the lattice spacing. There it is shown that at NLO the lattice spacing corrections to the $I = 2$, $I_3 = \pm 2$ scattering lengths are proportional to $\cos(\omega)$, where ω is the twist angle. Thus at maximal twist, $\omega = \pi/2$, the explicit discretization errors vanish exactly, and the scattering length can be simply represented by the continuum NLO χPT formula [52, 53].

As suggested in Refs. [37, 38], we perform the chiral extrapolation of $m_\pi a_{\pi\pi}^{I=2}$ in terms of m_π/f_π instead of m_π. Additionally, the χPT renormalization scale is fixed as $\mu = f_{\pi,\mathrm{phy}}$. The resulting NLO expression is then

$$m_\pi a_{\pi\pi}^{I=2} = -\frac{m_\pi^2}{8\pi f_\pi^2}\left\{1 + \frac{m_\pi^2}{16\pi^2 f_\pi^2}\left[3\ln\frac{m_\pi^2}{f_\pi^2} - 1 - l_{\pi\pi}^{I=2}(\mu = f_{\pi,\mathrm{phy}})\right]\right\}, \quad (4)$$

where $l_{\pi\pi}^{I=2}(\mu)$ is related to the Gasser-Leutwyler coefficients $\bar{l}_i$ as [54]

$$l_{\pi\pi}^{I=2}(\mu) = \frac{8}{3}\bar{l}_1 + \frac{16}{3}\bar{l}_2 - \bar{l}_3 - 4\bar{l}_4 + 3\ln\frac{m_{\pi,\mathrm{phy}}^2}{\mu^2}.$$

It is important to note that extrapolating in m_π/f_π instead of simply m_π does indeed change the expression for $m_\pi a_{\pi\pi}^{I=2}$ but only at the next-to-next-to-leading order (NNLO). The advantage of this form is that m_π/f_π is calculated

directly on the lattice with small errors and the chiral extrapolation does not require fixing a physical value for the lattice spacing.

We now fit our lattice results for $m_\pi a_{\pi\pi}^{I=2}$ from Tab. 1 to the functional form in Eq. 4 in order to extrapolate $m_\pi a_{\pi\pi}^{I=2}$ to the physical point and also extract the low energy constant $l_{\pi\pi}^{I=2}(\mu = f_{\pi,\mathrm{phy}})$. The calculated values for the scattering length and the resulting χPT fit curve are shown in Fig. 2. In the same figure,

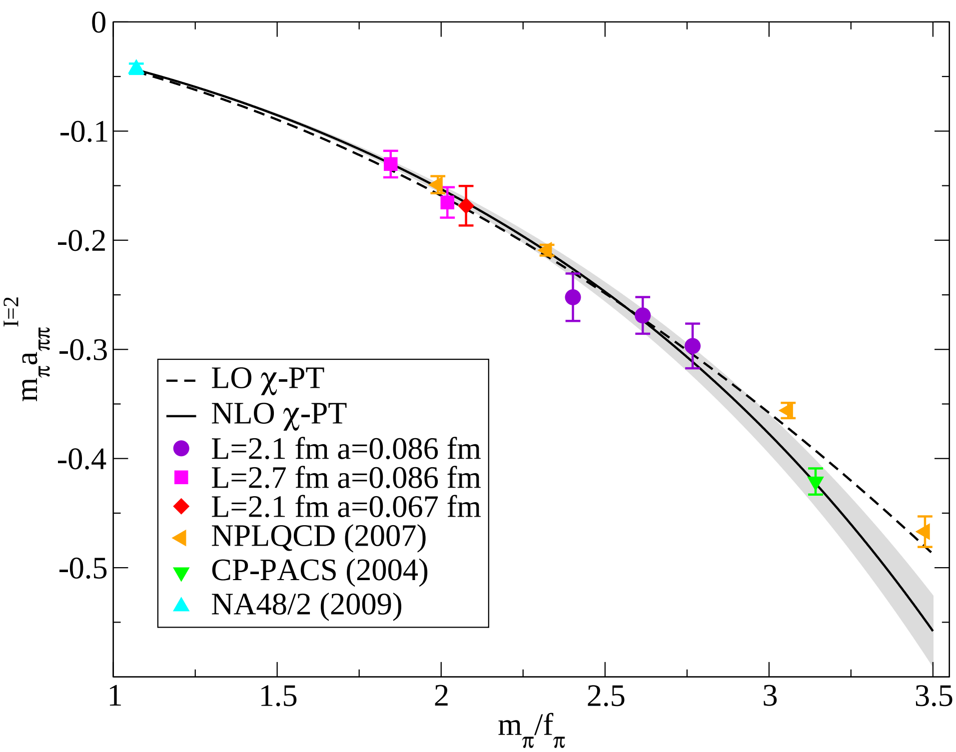

Fig. 2. Chiral extrapolation for the I=2 pion-pion scattering length. The results in this work are shown together with the lattice calculations of NPLQCD [37, 38] and CP-PACS [36] and the direct measurement from NA48/2 at CERN [7].

we also provide a comparison to the lattice results of NPLQCD [37, 38] and CP-PACS [36] and the direct measurement from NA48/2 at CERN [7]. We find general agreement between our calculation and the results of NPLQCD at similar pion masses. In particular, the agreement between our results and NPLQCD suggests that the effect of the missing strange quark in our current calculation is small. Additionally, the ongoing effort of ETMC to include the dynamical effects of both the strange and charm quark [55, 56] will allow us to directly address this issue.

To highlight the impact of the NLO terms in the χPT description of the pion mass dependence of $m_\pi a_{\pi\pi}^{I=2}$ and to understand the role of yet higher order terms, we show the difference between the lattice calculations of the scattering length and the LO χPT prediction in Fig. 3. We find that the scattering lengths statistically agree with the LO χPT result for all lattice calculations

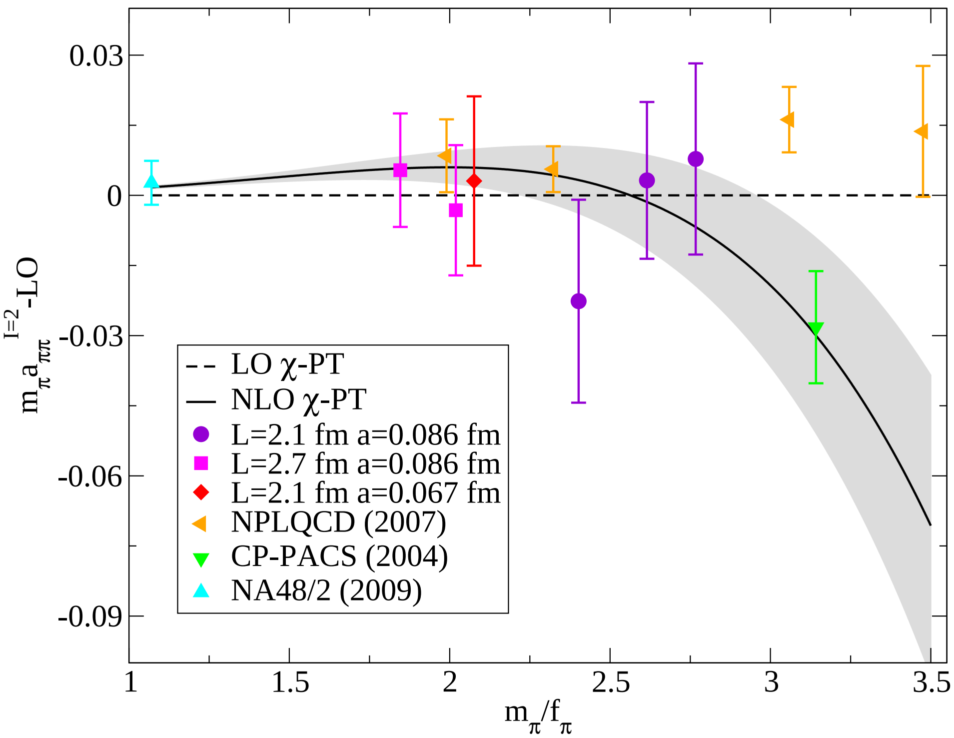

Fig. 3. Difference between the lattice calculation of the scattering lengths and the LO χPT prediction. The scattering lengths agree statistically with the LO χPT prediction for $m_\pi = 270$ MeV to 485 MeV.

with $m_\pi < 500$ MeV. Accordingly, the NLO χPT functional form provides a reasonable description of the lattice results in the same region of m_π. As a further check, we fit our calculations to the NNLO form for $m_\pi a_{\pi\pi}^{I=2}$ [4, 54] and found $m_\pi a_{\pi\pi}^{I=2} = -0.041\,(12)$ at the physical point. The statistical error is large, as one would expect given that our results already agree statistically with the LO χPT form, but the resulting NNLO extrapolation of $m_\pi a_{\pi\pi}^{I=2}$ does agree with the NLO fit. Given the size of the statistical errors, we are unable to make any meaningful estimate of the NNLO LECs, however, the effects from truncating the χPT series to NLO is included in our estimate of systematic errors.

The systematic error on the extrapolated value of $m_\pi a_{\pi\pi}^{I=2}$ and $l_{\pi\pi}^{I=2}$ has several components. First, the systematic errors of the $m_\pi a_{\pi\pi}^{I=2}$ that we obtain for each ensemble are propagated through the chiral extrapolation. This is accomplished by again collecting all fit ranges for each ensemble with $\chi^2/\mathrm{dof} < 2$ as earlier. This gives approximately 10^{10} χPT fits from which we randomly choose 2000 to sample the distribution of the extrapolated values of $m_\pi a_{\pi\pi}^{I=2}$. As for the individual $m_\pi a_{\pi\pi}^{I=2}$, we use the distribution method to determine an estimate of the systematic error due to the fit ranges from each ensemble. The second systematic uncertainty arises from the chiral fit itself. This is estimated by taking the difference in the extrapolated values from the NLO χPT fit to all six and just the lightest five ensembles. Finally, the extrapolation

to the physical point requires the experimental value for m_π/f_π. The experimental error on this quantity introduces an error that is nearly 50% of the corresponding statistical error and hence is also included. All three effects are added in quadrature to form the total estimated systematic error. Using the latest PDG [57] values of $m_{\pi^+} = 139.5702(4)$ MeV and $f_{\pi^+} = 130.4(2)$ MeV to determine the physical limit, we obtain the final result

$$m_\pi a_{\pi\pi}^{I=2} = -0.04385\,(28)(38) \quad \text{and} \quad l_{\pi\pi}^{I=2}(\mu = f_{\pi,\text{phy}}) = 4.65\,(.85)(1.07)\,.$$

This agrees with the previously mentioned results: the lattice calculation from NPLQCD [37, 38], the so-called CGL analysis [3, 4] and the E865 [2] and NA48/2 [7] measurements and represents agreement among the experimental and theoretical determinations of $m_\pi a_{\pi\pi}^{I=2}$ at the 1% level.

This accuracy of 1% must be understood as a combined theoretical effort from lattice QCD and chiral perturbation theory. The quantity $m_\pi a_{\pi\pi}^{I=2}$, as well as $a_{\pi\pi}^{I=2}$ itself, vanishes in the chiral limit. This significantly constrains the chiral extrapolation of $m_\pi a_{\pi\pi}^{I=2}$. In particular, $m_\pi a_{\pi\pi}^{I=2}$ is uniquely predicted in terms of m_π/f_π at LO and depends only on one unknown constant, $l_{\pi\pi}^{I=2}$, at NLO. This makes the chiral extrapolation of lattice results particularly accurate. Thus the 6% to 11% accurate results for the lattice calculation extrapolate to a 1% accurate determination of $m_\pi a_{\pi\pi}^{I=2}$. The final result differs from the LO χPT prediction by only a few percent, but to illustrate the power of combining lattice QCD and χPT, we note that the difference between $m_\pi a_{\pi\pi}^{I=2}$ and the LO result is $0.00173\,(47)$, which represents a 3.7σ shift that is due to the inclusion of the NLO effects as determined by matching directly to lattice QCD.

Chiral perturbation theory plays a strong role in obtaining $m_\pi a_{\pi\pi}^{I=2}$ accurately, but it alone can not determine $l_{\pi\pi}^{I=2}$. Only in combination with the lattice results can we calculate $l_{\pi\pi}^{I=2} = 4.65\,(1.37)$. This calculation is just under 30% accurate, however, as we explain shortly, this easily exceeds the experimental determinations of this quantity. The experimental and phenomenological results for $m_\pi a_{\pi\pi}^{I=2}$ at the physical point can be converted into a result for $l_{\pi\pi}^{I=2}$ at NLO. A simple analysis gives the following for $l_{\pi\pi}^{I=2}$: 3.0 ± 3.1 (CGL), 0.0 ± 10.3 (E865 with χPT) and 3.0 ± 2.8 (NA48/2 with χPT). This comparison demonstrates the particular advantage of lattice calculations arising from the ability to vary the underlying quark masses of QCD.

5 Conclusion

We have calculated the s-wave pion-pion scattering length in the isospin $I = 2$ channel using the two-flavor maximally twisted mass lattice QCD configurations from ETMC. The pion masses ranged from 270 MeV to 485 MeV and

the lattice spacing was $a = 0.086$ fm. A second lattice spacing of $a = 0.067$ fm was used to demonstrate the absence of large lattice artifacts. This is only a single check, but when combined with the fact that the calculation is accurate to $O(a^2)$ due to the properties of maximally twisted mass fermions, it suggests that the lattice spacing dependence is mild. Furthermore, discretization errors vanish from the $I = 2$, $I_3 = \pm 2$ channel at NLO, as shown by twisted mass χPT, hence we extrapolated our results for the scattering length to the physical limit using continuum χPT at NLO. We investigated various systematic effects, and we found for the scattering length at the physical point $m_\pi a_{\pi\pi}^{I=2} = -0.04385\,(28)(38)$ and for the low energy constant $l_{\pi\pi}^{I=2}(\mu = f_{\pi,\mathrm{phy}}) = 4.65\,(.85)(1.07)$. These results are in good agreement with the previous lattice calculation from NPLQCD, the experimental determinations from E865 at BNL and from NA48/2 at CERN and the CGL analysis using various theoretical and experimental inputs.

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